wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 06:28 PM EST

PDB ID	:	6MU2
EMDB ID	:	EMD-9244
Title	:	Structure of full-length IP3R1 channel in the Apo-state
Authors	:	Serysheva, I.I.; Fan, G.; Baker, M.R.; Wang, Z.; Seryshev, A.; Ludtke, S.J.; Baker, M.L.
Deposited on	:	2018-10-22
Resolution	:	3.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

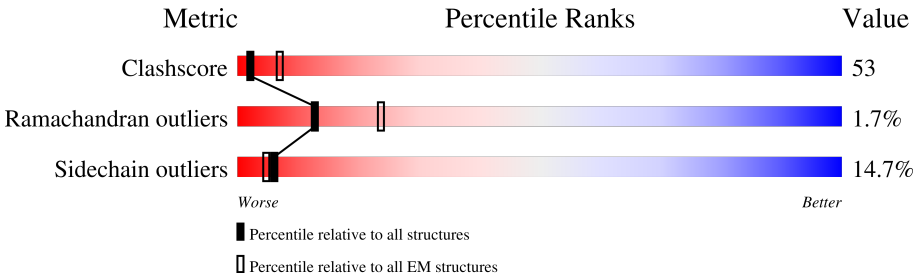
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2750	16% 54% 19% 5% • 21%
1	B	2750	16% 54% 19% 5% • 21%
1	C	2750	16% 54% 19% 5% • 21%
1	D	2750	16% 54% 19% 5% • 21%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 51404 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

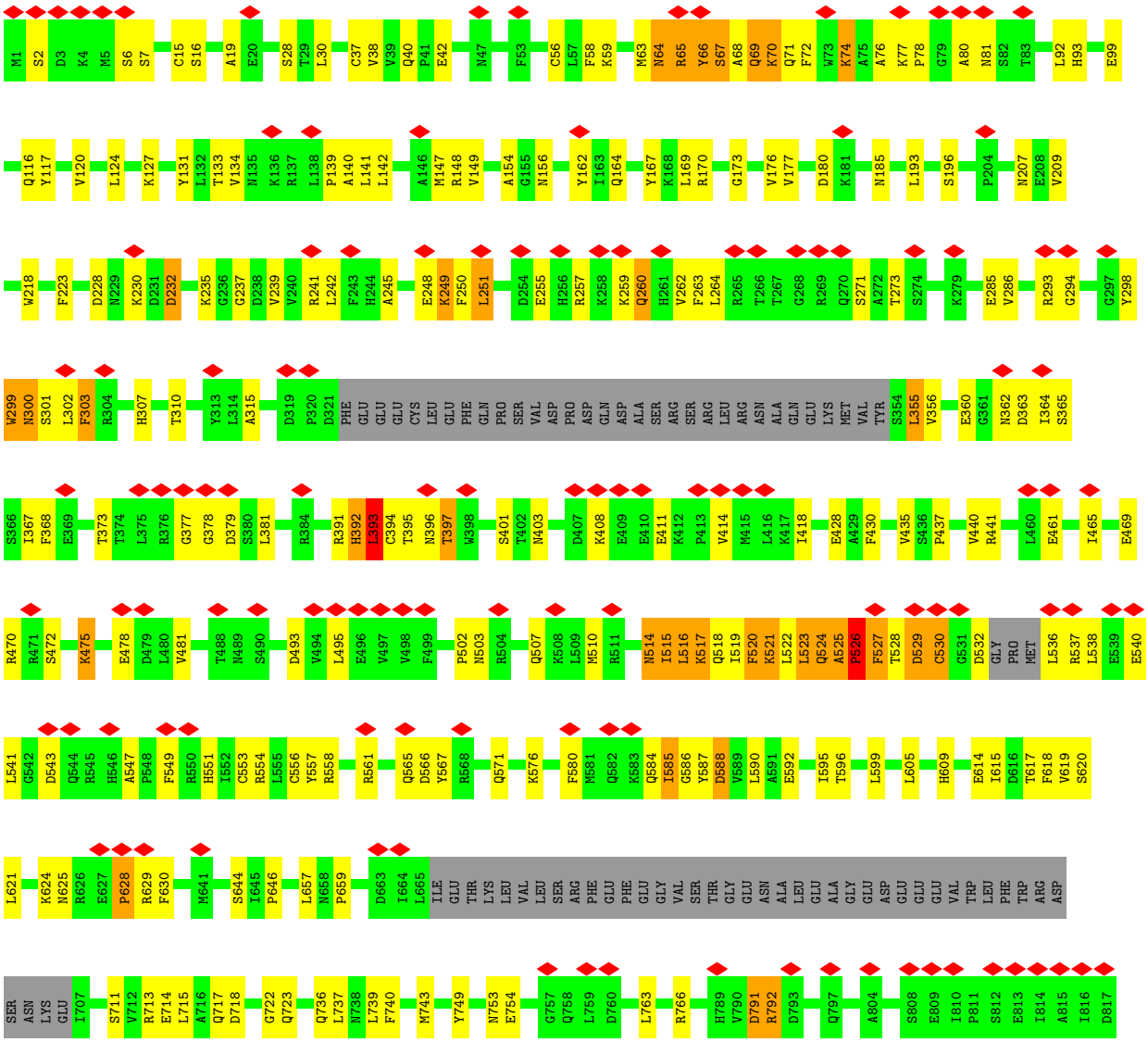
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	2170	12851	7584	2562	2660	45	0	0
1	A	2170	12851	7584	2562	2660	45	0	0
1	D	2170	12851	7584	2562	2660	45	0	0
1	C	2170	12851	7584	2562	2660	45	0	0

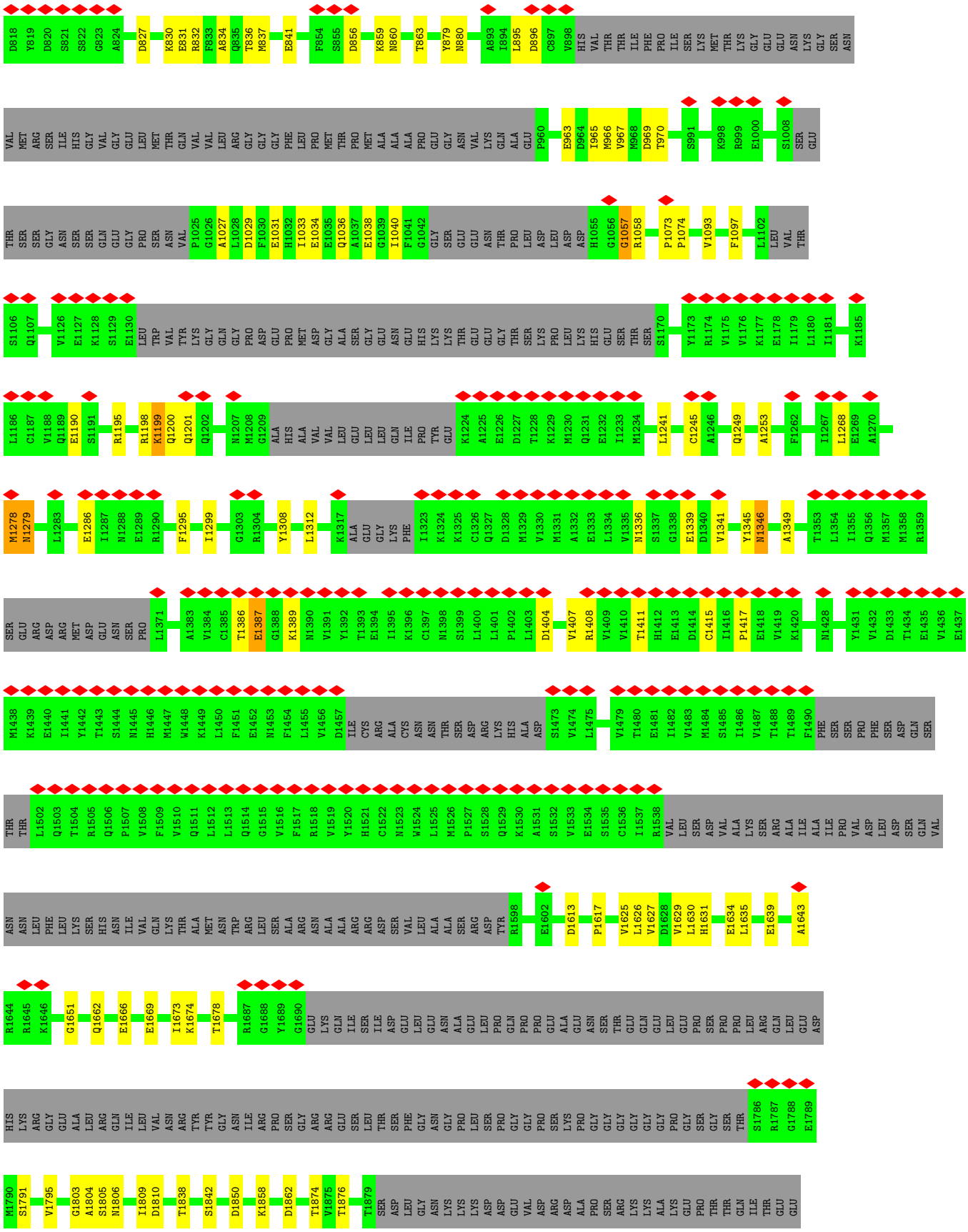
3 Residue-property plots (i)

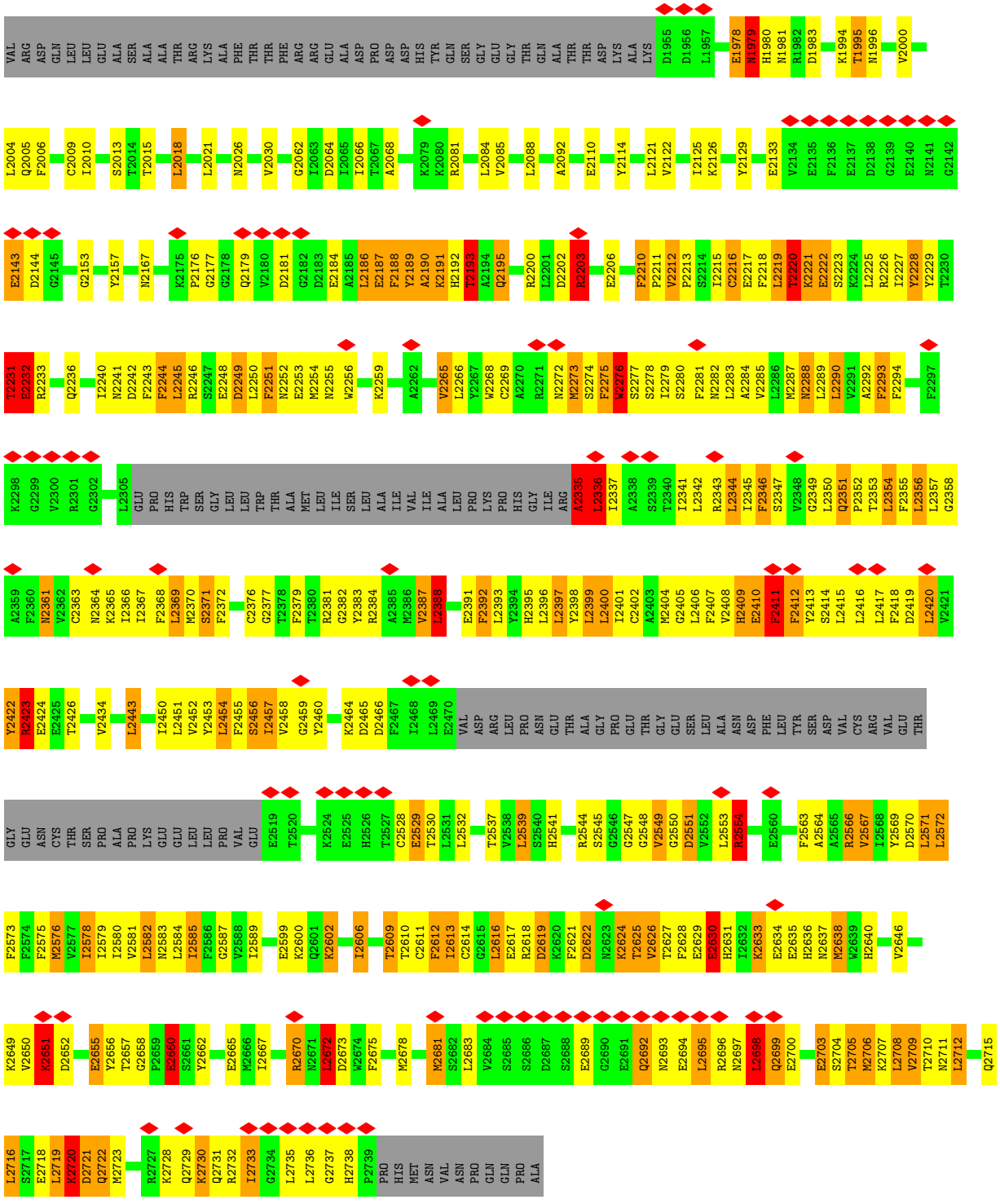
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain B:

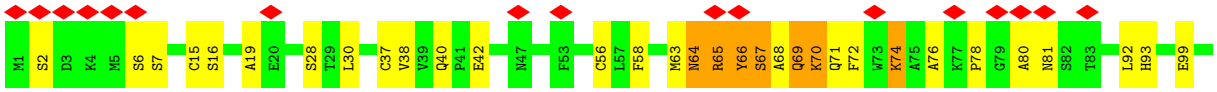


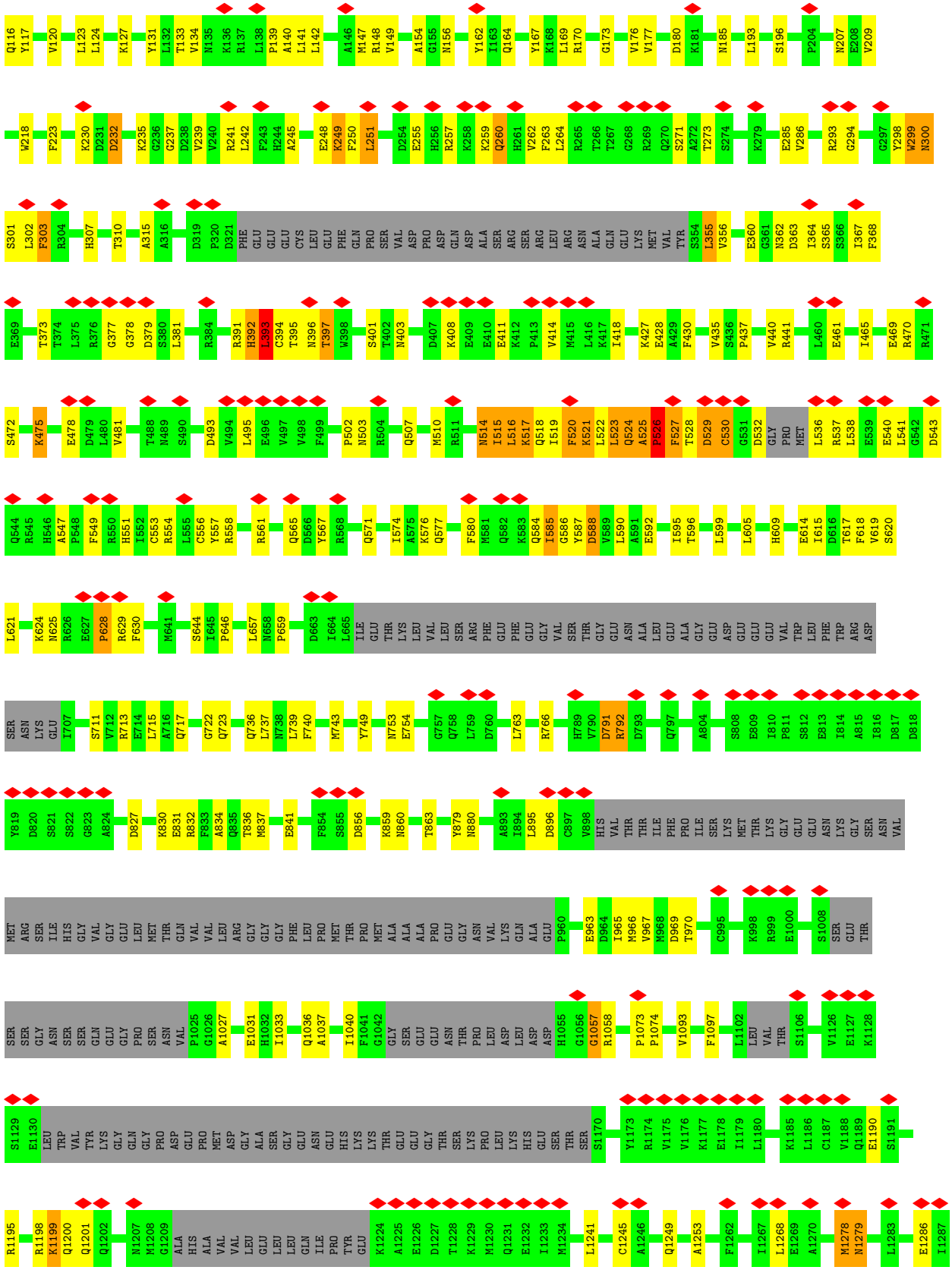

D818 Y819 D820 S821 S822 G823 A824 D827 K830 E831 R832 F833 A834 Q835 T836 M837 E841 F854 S855 D856 K859 N860 T863 Y879 N880 A893 I894 L895 D896 C897 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN
VAL MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 S991 K998 R999 E1000 S1008 SER GLU
THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 L1028 D1029 F1030 E1031 H1032 I1033 E1034 E1035 Q1036 A1037 E1038 G1039 I1040 F1041 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 G1057 R1058 P1073 P1074 V1093 F1097 L1102 LEU VAL THR
S1106 Q1107 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1173 R1174 V1175 V1176 K1177 E1178 I1179 L1180 I1181 K1185
L1186 C1187 V1188 Q1189 E1190 S1191 R1195 R1198 K1199 Q1200 Q1201 Q1202 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 L1241 C1245 A1246 Q1249 A1253 F1262 I1267 L1268 E1269 A1270
M1278 N1279 L1283 E1286 I1287 N1288 E1289 R1290 F1295 I1299 G1303 R1304 Y1308 L1312 K1317 ALA GLU GLY LYS PHE I1323 K1324 K1325 C1326 Q1327 D1328 M1329 V1330 M1331 A1332 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 Y1345 N1346 A1349 T1353 L1354 I1355 Q1356 M1357 M1358 R1359
SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 A1383 V1384 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 N1428 Y1431 V1432 D1433 T1434 E1435 V1436 E1437
M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO PHE SER ASP GLN SER
THR THR L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN VAL
ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 E1602 D1613 P1617 V1625 L1626 V1627 D1628 V1629 L1630 H1631 E1634 L1635 E1639 A1643
R1644 R1645 K1646 G1651 Q1662 E1666 E1669 T1673 K1674 T1678 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO PRO LEU ARG GLN LEU GLU ASP
HIS LYS ARG GLY GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY PRO GLY SER GLY SER THR S1786 R1787 G1788 E1789
M1790 S1791 V1795 G1803 A1804 S1805 N1806 I1809 D1810 T1838 S1842 D1850 K1858 D1862 T1874 V1875 T1876 T1879 SER ASP LEU GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU

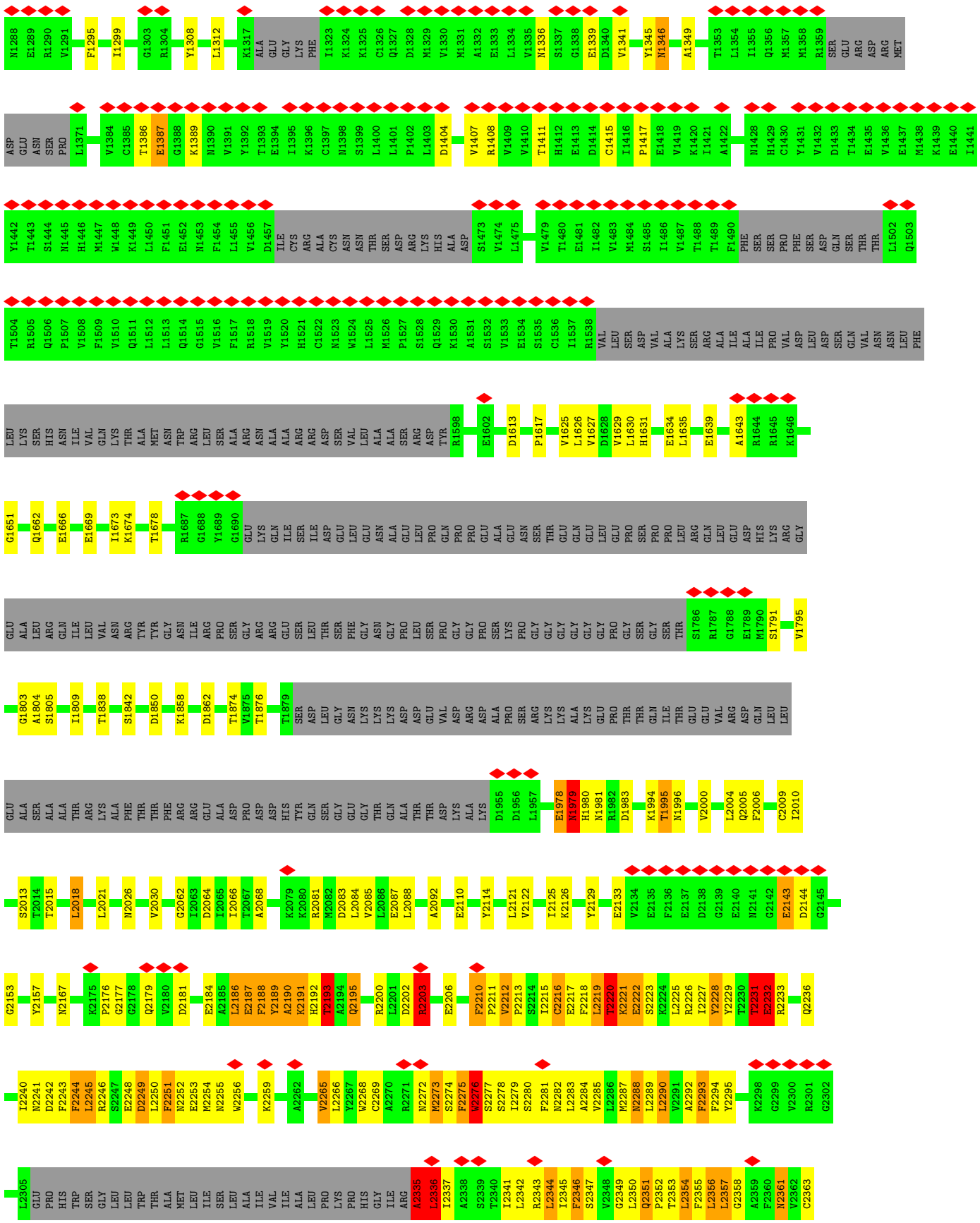


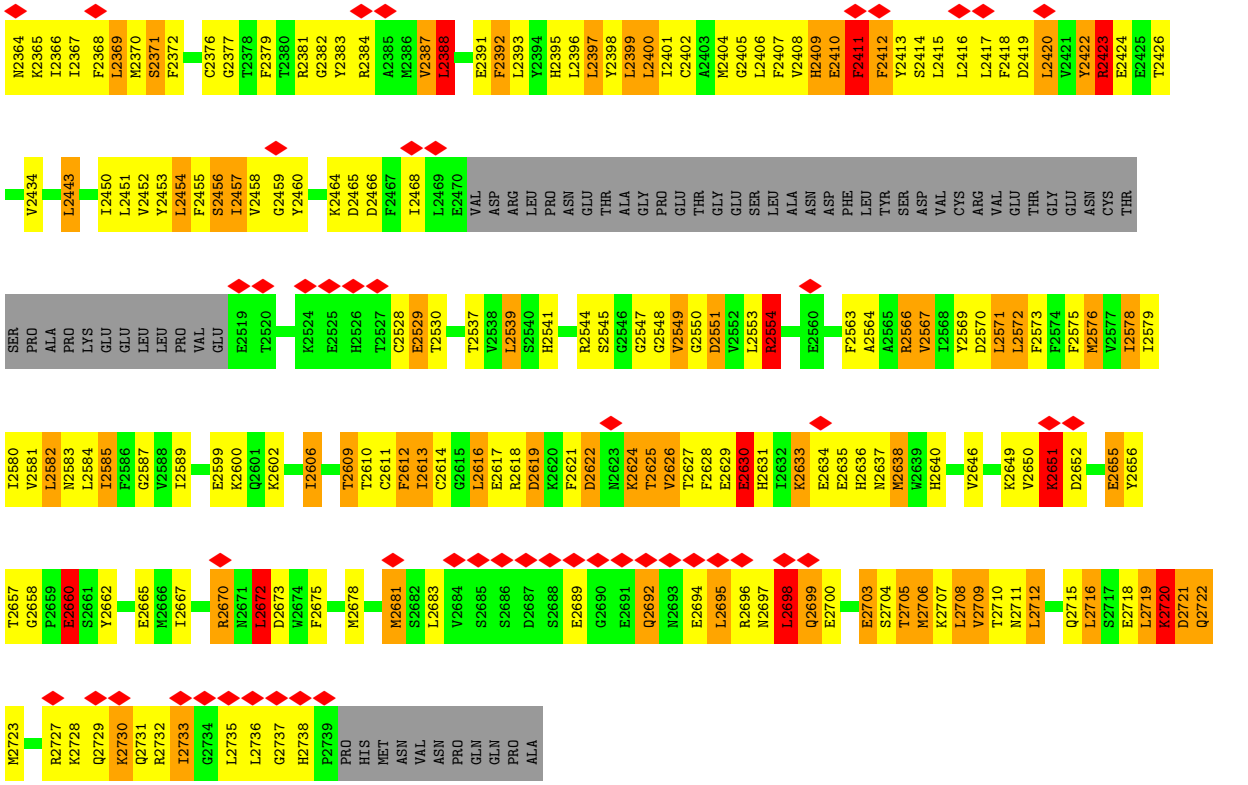
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain A:



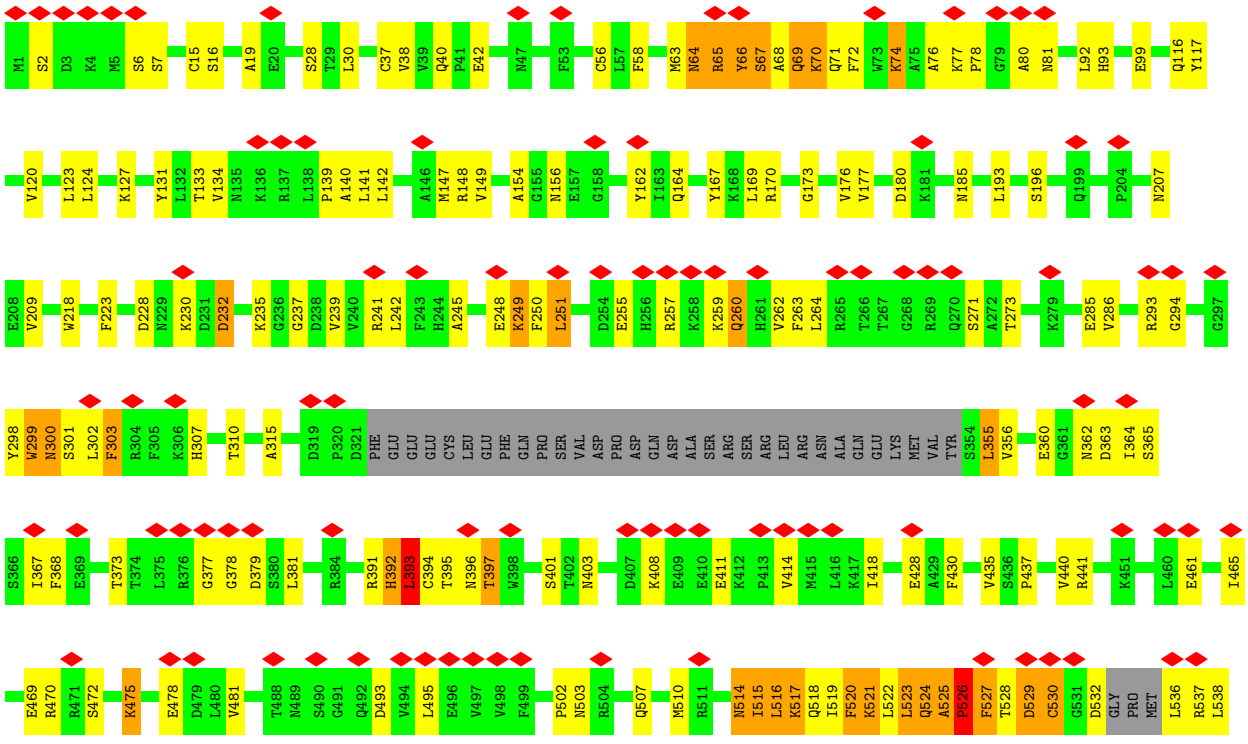

Q116 Y117 V120 L123 L124 K127 Y131 L132 T133 V134 N135 K136 R137 L138 P139 A140 L141 L142 A146 M147 R148 V149 A154 G155 N156 Y162 I163 Q164 Y167 K168 L169 R170 G173 V176 V177 D180 K181 N185 L193 S196 P204 N207 E208 V209
W218 F223 K230 D231 D232 K235 G236 G237 D238 V239 V240 R241 L242 F243 H244 A245 E248 K249 F250 L251 D254 E255 H256 R257 K258 K259 Q260 H261 V262 F263 L264 R265 T266 T267 G268 R269 Q270 S271 A272 T273 S274 K279 E285 V286 R293 G294 G297 Y298 W299 N300
S301 L302 F303 R304 H307 T310 A315 A316 D319 P320 D321 PHE GLU GLU GLU CYS LEU GLU PHE GLN PRO SER VAL ASP PRO ASP GLN ASP ALA SER ARG SER ARG LEU ARG ASN ALA GLN GLU LYS MET VAL TYR S354 L355 V356 E360 G361 N362 D363 I364 S365 S366 I367 F368
E369 T373 T374 L375 R376 G377 G378 D379 S380 L381 R384 R391 H392 L393 C394 T395 N396 T397 W398 S401 T402 N403 D407 K408 E409 E410 E411 K412 P413 V414 M415 L416 K417 I418 K427 E428 A429 F430 V435 S436 P437 V440 R441 L460 E461 I465 E469 R470 R471
S472 K475 E478 D479 L480 V481 T488 N489 S490 D493 V494 L495 E496 V497 V498 F499 P502 N503 R504 Q507 M510 R511 N514 I515 L516 K517 Q518 I519 F520 K521 L522 L523 Q524 A525 P526 F527 T528 D529 C530 G531 D532 GLY PRO MET L536 R537 L538 E539 E540 L541 G542 D543
Q544 R545 H546 A547 P548 F549 R550 H551 I552 C553 R554 I555 C556 Y557 R558 R561 Q565 D566 Y567 R568 Q571 I574 A575 K576 Q577 F580 M581 Q582 K583 Q584 I585 G586 Y587 D588 V589 L590 A591 E592 I595 T596 L599 L605 H609 E614 I615 D616 T617 F618 V619 S620
L621 K624 N625 R626 E627 P628 R629 F630 M641 S644 I645 P646 L657 N658 P659 D663 I664 L665 ILE GLU THR LYS LEU VAL LEU SER ARG PHE GLU PHE GLU GLY VAL SER THR GLY GLU ASN ALA LEU GLU ALA GLY GLU ASP GLU GLU GLU VAL TRP LEU PHE TRP ARG ASP
SER ASN LYS GLU I707 S711 V712 R713 E714 L715 A716 Q717 G722 Q723 Q736 L737 N738 L739 F740 M743 Y749 N753 E754 G757 Q758 L759 D760 L763 R766 H789 V790 D791 R792 D793 Q797 A804 S808 E809 I810 P811 S812 E813 I814 A815 A816 D817 D818
Y819 D820 S821 S822 G823 A824 D827 K830 E831 R832 F833 A834 Q835 T836 M837 E841 F854 S855 D856 K859 N860 T863 Y879 N880 A893 I894 L895 D896 C897 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN LYS GLY SER ASN VAL
MET ARG SER ILE HIS GLY VAL GLY GLU LEU MET THR GLN VAL VAL LEU ARG GLY GLY GLY PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 C995 K998 R999 E1000 S1008 SER GLU THR
SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 E1031 H1032 I1033 Q1036 A1037 I1040 F1041 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 G1057 R1058 P1073 P1074 V1093 F1097 L1102 LEU VAL THR S1106 V1126 E1127 K1128
S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1173 R1174 V1175 V1176 K1177 E1178 I1179 L1180 K1185 L1186 C1187 V1188 Q1189 E1190 S1191
R1195 R1198 K1199 Q1200 Q1201 Q1202 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 L1241 C1245 A1246 Q1249 A1253 F1262 I1267 L1268 E1269 A1270 M1278 N1279 L1283 E1286 I1287

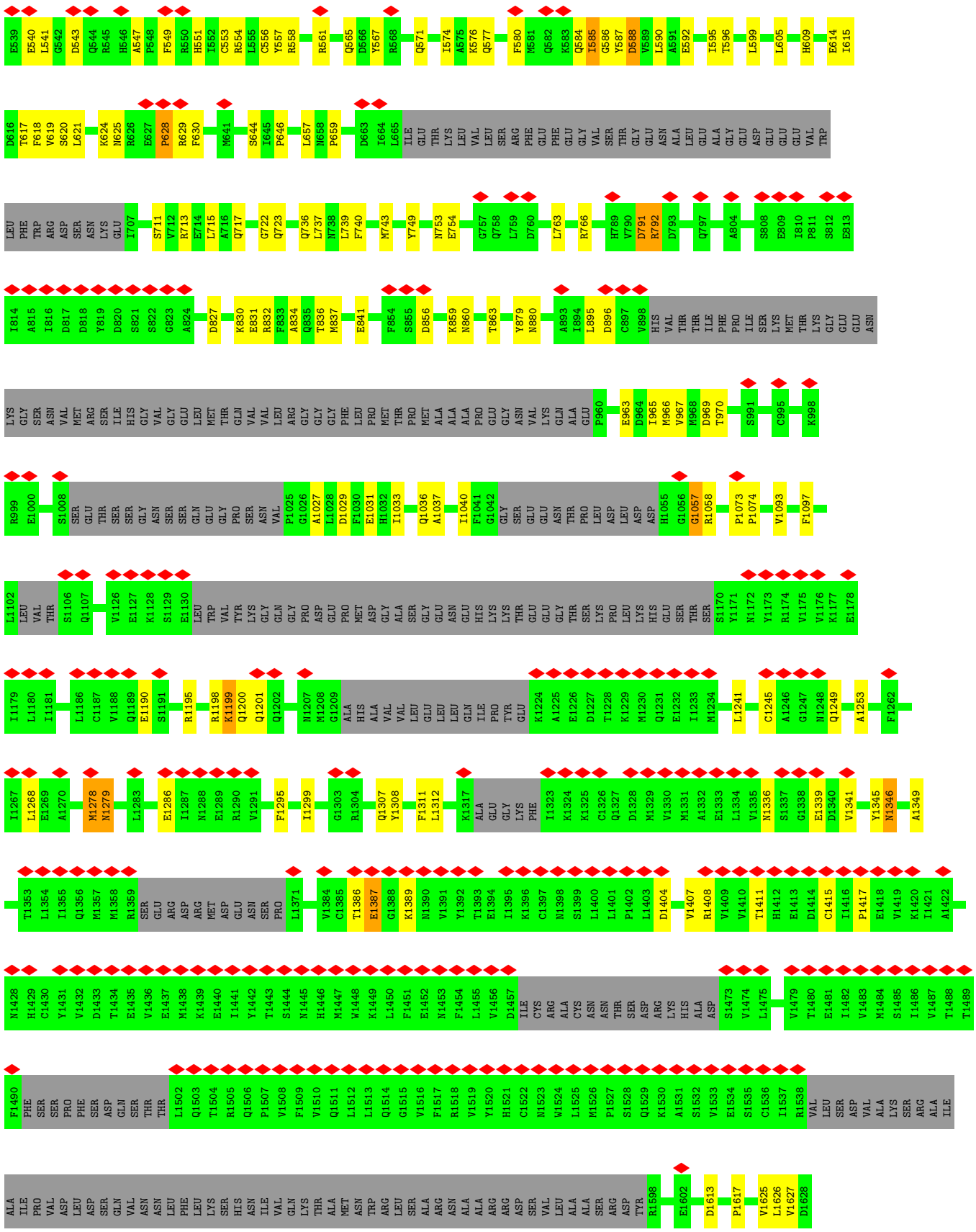

N1288 E1289 R1290 V1291 F1295 I1299 G1303 R1304 Y1308 L1312 K1317 ALA GLU GLY LYS PHE I1323 K1324 K1325 C1326 Q1327 D1328 M1329 V1330 M1331 A1332 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 Y1345 N1346 A1349 T1353 L1354 I1355 Q1356 M1357 M1358 R1359 SER GLU ARG ASP ARG MET
ASP GLU ASN SER PRO L1371 V1384 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 N1428 H1429 C1430 Y1431 V1432 D1433 T1434 E1435 V1436 E1437 M1438 K1439 E1440 I1441
Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO PHE SER ASP GLN SER THR THR L1502 Q1503
T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP LEU ASP SER GLN SER GLN VAL ASN ASN LEU PHE
LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 E1602 D1613 P1617 V1625 L1626 V1627 D1628 V1629 L1630 H1631 E1634 L1635 E1639 A1643 R1644 R1645 K1646
G1651 Q1662 E1666 E1669 I1673 K1674 T1678 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO PRO LEU ARG GLN LEU GLU ASP HIS LYS ARG GLY
GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY GLY PRO GLY SER GLY SER THR S1786 R1787 G1788 E1789 M1790 S1791 V1795
G1803 A1804 S1805 I1809 T1838 S1842 D1850 K1858 D1862 T1874 V1875 T1876 T1879 SER ASP LEU GLY GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE THR GLU GLU GLU VAL ARG ASP GLN LEU LEU
GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 L1957 E1978 N1979 H1980 N1981 R1982 D1983 K1994 T1995 N1996 V2000 L2004 Q2005 F2006 C2009 I2010
S2013 T2014 T2015 L2018 L2021 N2026 V2030 G2062 I2063 D2064 I2065 I2066 T2067 A2068 K2079 K2080 R2081 M2082 D2083 L2084 V2085 L2086 E2087 L2088 A2092 E2110 Y2114 L2121 V2122 I2125 K2126 Y2129 E2133 V2134 E2135 F2136 E2137 D2138 G2139 E2140 N2141 G2142 E2143 D2144 G2145
G2153 Y2157 N2167 K2175 P2176 G2177 G2178 Q2179 V2180 D2181 E2184 A2185 L2186 E2187 F2188 Y2189 A2190 K2191 H2192 T2193 A2194 Q2195 R2200 L2201 D2202 R2203 E2206 F2210 P2211 V2212 P2213 S2214 I2215 C2216 E2217 F2218 L2219 T2220 K2221 E2222 S2223 K2224 L2225 R2226 I2227 Y2228 Y2229 T2230 T2231 E2232 R2233 Q2236
I2240 N2241 D2242 F2243 F2244 L2245 R2246 S2247 E2248 D2249 L2250 F2251 N2252 E2253 M2254 N2255 W2256 K2259 A2262 V2265 L2266 Y2267 W2268 C2269 A2270 R2271 N2272 M2273 S2274 F2275 W2276 S2277 S2278 I2279 S2280 F2281 N2282 L2283 A2284 V2285 L2286 M2287 N2288 L2289 L2290 V2291 A2292 F2293 F2294 Y2295 K2298 G2299 V2300 R2301 G2302
L2305 GLU PRO HIS TRP SER GLY LEU LEU TRP THR ALA MET LEU ILE SER LEU ALA ILE VAL ILE ALA LEU PRO LYS PRO HIS GLY ILE ARG A2335 L2336 I2337 A2338 S2339 T2340 I2341 L2342 R2343 L2344 I2345 F2346 S2347 V2348 G2349 L2350 Q2351 P2352 T2353 L2354 F2355 L2356 L2357 G2358 A2359 F2360 N2361 V2362 C2363

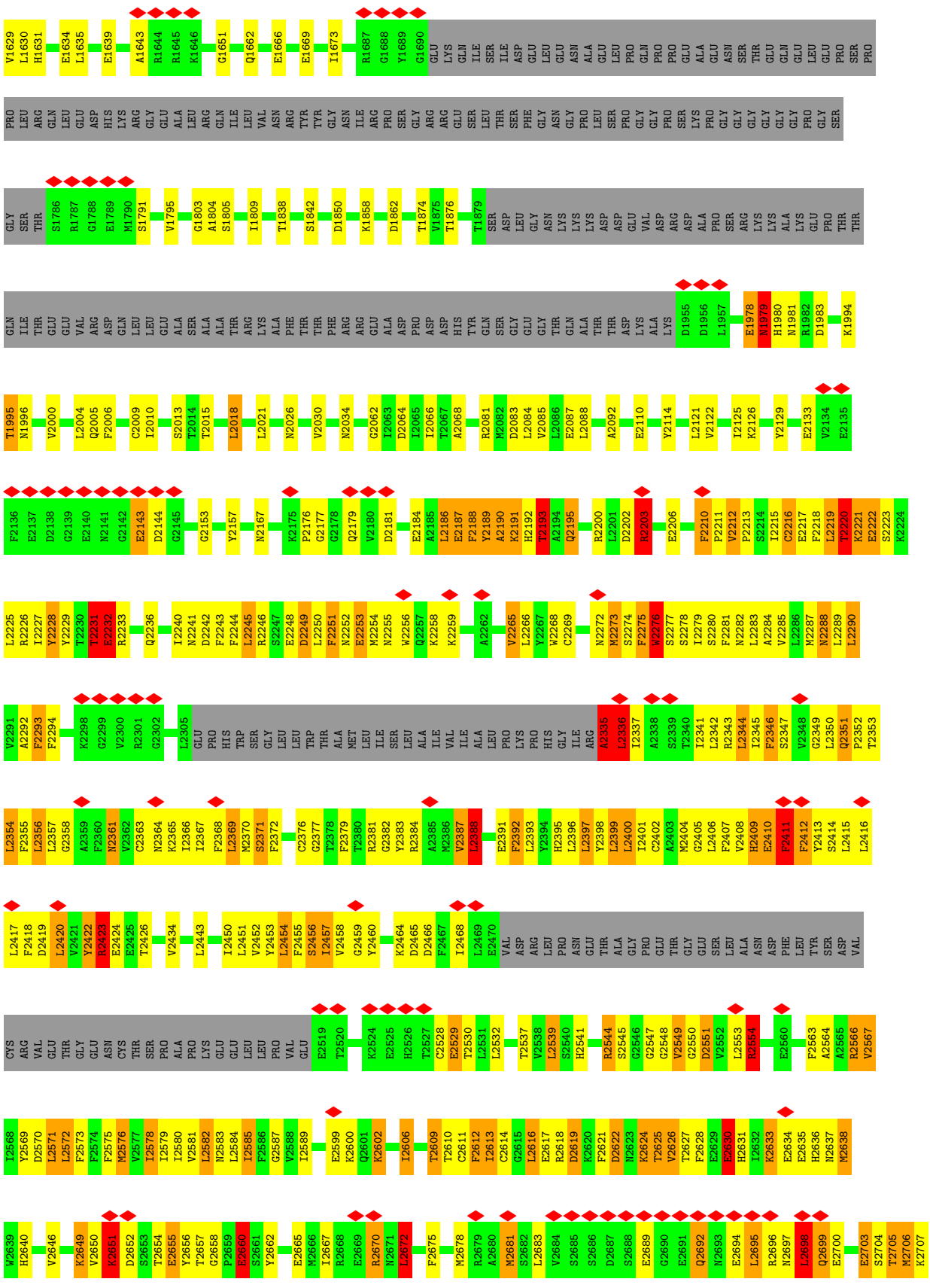


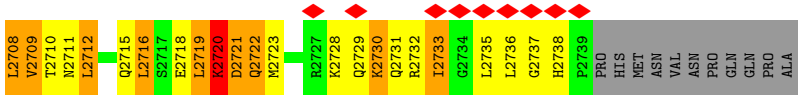
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain D:



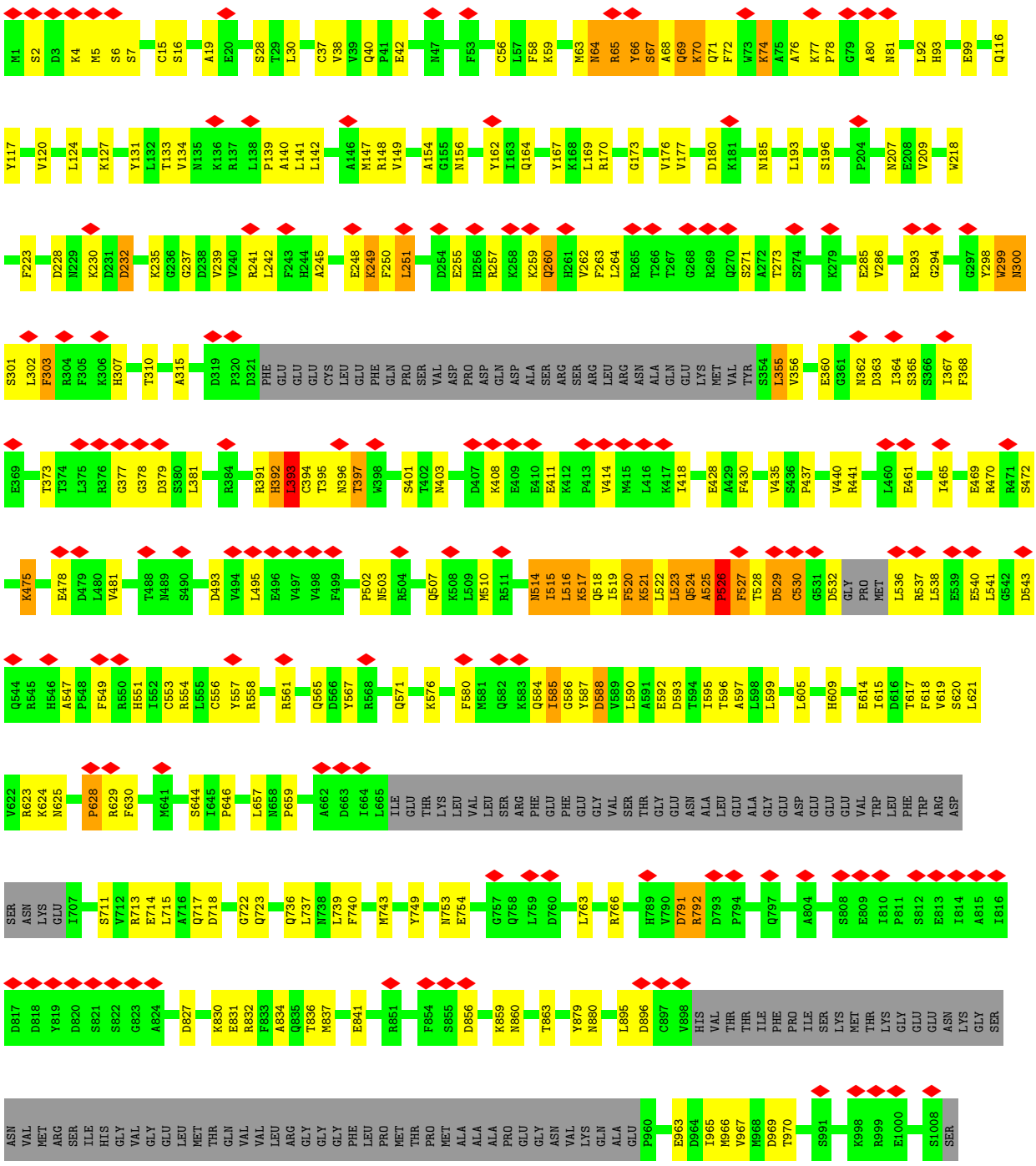

E539 E540 L541 G542 D543 Q544 R545 H546 A547 P548 F549 R550 H551 I552 C553 R554 L555 C556 Y557 R558 R561 Q565 D566 Y567 R568 Q571 I574 A575 K576 Q577 F580 M581 Q582 K583 Q584 I585 G586 Y587 D588 V589 L590 A591 E592 I595 T596 L599 L605 H609 E614 I615
D616 T617 F618 V619 S620 L621 K624 N625 R626 E627 P628 R629 F630 M641 S644 T645 P646 L657 H658 P659 D663 I664 L665 ILE GLU THR LYS LEU VAL LEU SER ARG PHE GLU PHE GLU GLY VAL SER THR GLY GLU ASN ALA LEU GLU ALA GLY GLU ASP GLU GLU GLU VAL TRP
LEU PHE TRP ARG ASP SER ASN LYS GLU I707 S711 V712 R713 E714 L715 A716 Q717 G722 Q723 Q736 L737 N738 L739 F740 M743 Y749 N753 E754 G757 Q758 L759 D760 L763 R766 H789 V790 D791 R792 D793 Q797 A804 S808 E809 I810 P811 S812 E813
I814 A815 I816 D817 D818 Y819 D820 S821 S822 G823 A824 D827 K830 E831 R832 F833 A834 Q835 T836 M837 E841 F854 S855 D856 K859 N860 T863 Y879 N880 A893 I894 L895 D896 C897 V898 HIS VAL THR THR ILE PHE PRO ILE SER LYS MET THR LYS GLY GLU GLU ASN
LYS GLY SER ASN VAL MET ARG SER ILE HIS GLY VAL GLU GLU LEU MET THR GLN VAL VAL VAL LEU ARG GLY GLY GLY PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLU GLY ASN VAL LYS GLN ALA GLU P960 E963 D964 I965 M966 V967 M968 D969 T970 S991 C995 K998
R999 E1000 S1008 SER GLU THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 ARG GLY GLY GLY PHE LEU PRO MET THR PRO MET ALA ALA ALA PRO GLU GLU GLY ASN VAL LYS GLN ALA GLU H1055 G1056 G1057 R1058 P1073 P1074 V1093 F1097
L1102 LEU VAL THR S1106 Q1107 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178
I1179 L1180 I1181 L1186 C1187 V1188 Q1189 E1190 S1191 R1195 R1198 K1199 Q1200 Q1201 Q1202 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 L1241 C1245 A1246 G1247 N1248 Q1249 A1253 F1262
I1267 L1268 E1269 A1270 M1278 N1279 L1283 E1286 I1287 N1288 E1289 R1290 V1291 F1295 I1299 G1303 R1304 Q1307 Y1308 F1311 L1312 K1317 ALA GLU GLY LYS PHE I1323 K1324 K1325 C1326 Q1327 D1328 M1329 V1330 M1331 A1332 E1333 L1334 V1335 N1336 S1337 C1338 E1339 D1340 V1341 Y1345 N1346 A1349
T1353 L1354 I1355 Q1356 M1357 M1358 R1359 SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 V1384 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422
N1428 H1429 C1430 Y1431 V1432 D1433 T1434 E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489
F1490 PHE SER SER PRO PHE SER ASP GLN SER THR THR L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE
ALA ILE PRO VAL ASP LEU ASP SER GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 E1602 D1613 P1617 V1625 L1626 V1627 D1628

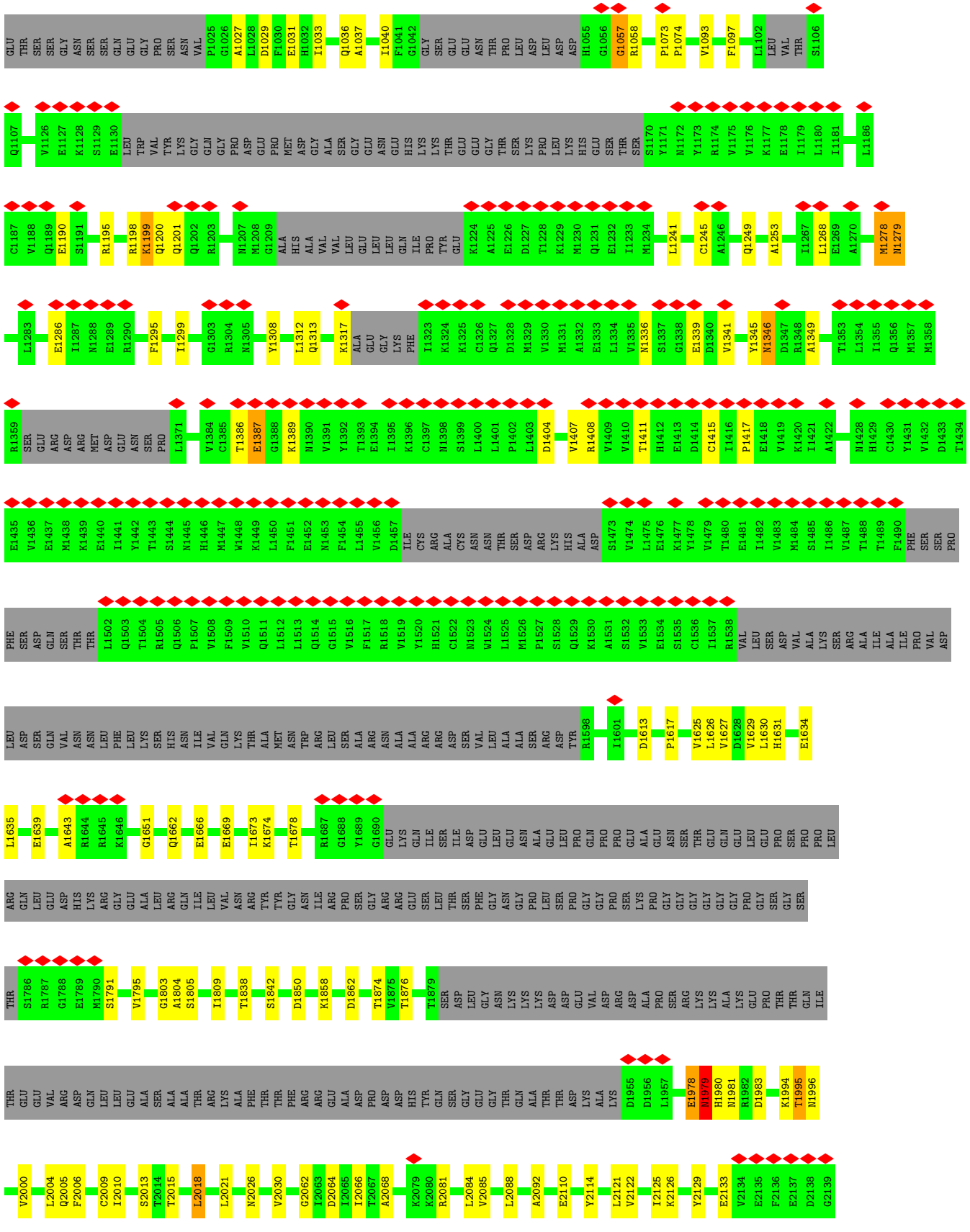

V1629 L1630 H1631 E1634 L1635 E1639 A1643 R1644 R1645 K1646 G1651 Q1662 E1666 E1669 I1673 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO
PRO LEU ARG GLN LEU GLU ASP HIS LYS ARG GLY GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY GLY PRO GLY SER
GLY SER THR S1786 R1787 G1788 E1789 M1790 S1791 V1795 G1803 A1804 S1805 I1809 T1838 S1842 D1850 K1858 D1862 T1874 V1875 T1876 T1879 SER ASP LEU GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR
GLN ILE THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 L1957 E1978 N1979 H1980 N1981 R1982 D1983 K1994
T1995 N1996 V2000 L2004 Q2005 F2006 C2009 I2010 S2013 T2014 T2015 L2018 L2021 N2026 V2030 N2034 G2062 I2063 D2064 I2065 I2066 T2067 A2068 R2081 M2082 D2083 L2084 V2085 L2086 E2087 L2088 A2092 E2110 Y2114 L2121 V2122 I2125 K2126 Y2129 E2133 V2134 E2135
F2136 E2137 D2138 G2139 E2140 N2141 G2142 E2143 D2144 G2145 G2153 Y2157 N2167 K2175 P2176 G2177 G2178 Q2179 V2180 D2181 E2184 A2185 L2186 E2187 F2188 Y2189 A2190 K2191 H2192 T2193 A2194 Q2195 R2200 L2201 D2202 R2203 E2206 F2210 P2211 V2212 P2213 S2214 I2215 C2216 E2217 F2218 L2219 T2220 K2221 E2222 S2223 K2224
L2225 R2226 I2227 Y2228 Y2229 T2230 T2231 E2232 R2233 Q2236 I2240 N2241 D2242 F2243 F2244 L2245 R2246 S2247 E2248 D2249 L2250 F2251 N2252 E2253 M2254 N2255 W2256 Q2257 K2258 K2259 A2262 V2265 L2266 Y2267 W2268 C2269 N2272 M2273 S2274 F2275 W2276 S2277 S2278 I2279 S2280 F2281 N2282 L2283 A2284 V2285 L2286 M2287 N2288 L2289 L2290
V2291 A2292 F2293 F2294 K2298 G2299 V2300 R2301 G2302 L2305 GLU PRO HIS TRP SER GLY LEU LEU TRP THR ALA MET LEU ILE SER LEU ALA ILE VAL ILE ALA LEU PRO LYS PRO HIS GLY ILE ARG A2335 L2336 I2337 A2338 S2339 T2340 I2341 L2342 R2343 L2344 I2345 F2346 S2347 V2348 G2349 L2350 Q2351 P2352 T2353
L2354 F2355 L2356 L2357 G2358 A2359 F2360 N2361 V2362 C2363 N2364 K2365 I2366 I2367 F2368 L2369 M2370 S2371 F2372 C2376 G2377 T2378 F2379 T2380 R2381 G2382 Y2383 R2384 A2385 M2386 V2387 L2388 E2391 F2392 L2393 Y2394 H2395 L2396 L2397 Y2398 L2399 L2400 I2401 C2402 A2403 M2404 G2405 L2406 F2407 V2408 H2409 E2410 F2411 F2412 Y2413 S2414 L2415 L2416
L2417 F2418 D2419 L2420 V2421 Y2422 R2423 E2424 E2425 T2426 V2434 L2443 I2450 L2451 V2452 Y2453 L2454 F2455 S2456 I2457 V2458 G2459 Y2460 K2464 D2465 D2466 F2467 I2468 L2469 E2470 VAL ASP ARG LEU PRO ASN GLU THR ALA GLY PRO GLU THR GLY GLU SER LEU ALA ASN ASP PHE LEU TYR SER ASP VAL
CYS ARG VAL GLU THR GLY GLU ASN CYS THR SER PRO ALA PRO LYS GLU GLU LEU LEU PRO VAL GLU E2519 T2520 K2524 E2525 H2526 T2527 C2528 E2529 T2530 L2531 L2532 T2537 V2538 L2539 S2540 H2541 R2544 S2545 G2546 G2547 G2548 V2549 G2550 D2551 V2552 L2553 R2554 E2560 F2563 A2564 A2565 R2566 V2567
I2568 Y2569 D2570 L2571 L2572 F2573 F2574 F2575 M2576 V2577 I2578 I2579 I2580 V2581 L2582 N2583 L2584 I2585 F2586 G2587 V2588 I2589 E2599 K2600 Q2601 K2602 I2606 T2609 T2610 C2611 F2612 I2613 C2614 G2615 L2616 E2617 R2618 D2619 K2620 F2621 D2622 N2623 K2624 T2625 V2626 T2627 F2628 E2629 E2630 H2631 I2632 K2633 E2634 E2635 H2636 N2637 M2638
W2639 H2640 V2646 K2649 V2650 K2651 D2652 S2653 T2654 E2655 Y2656 T2657 G2658 P2659 E2660 S2661 Y2662 E2665 M2666 I2667 R2668 E2669 R2670 N2671 L2672 F2675 M2678 R2679 A2680 M2681 S2682 L2683 V2684 S2685 S2686 D2687 S2688 E2689 G2690 E2691 Q2692 N2693 E2694 L2695 R2696 N2697 L2698 Q2699 E2700 E2703 S2704 T2705 M2706 K2707

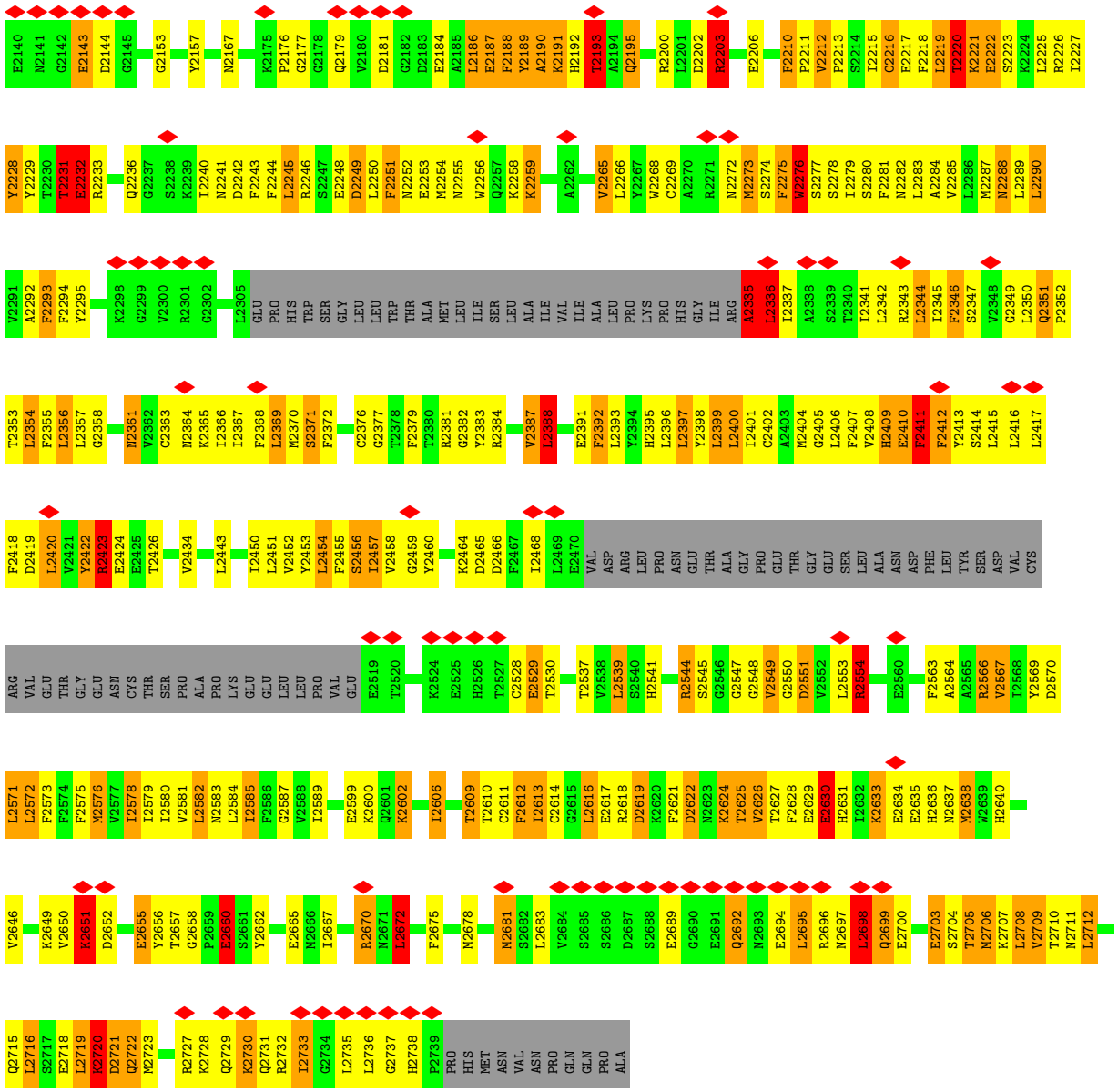


- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain C:




GLU THR SER SER GLY ASN SER SER GLN GLU GLY PRO SER ASN VAL P1025 G1026 A1027 L1028 D1029 F1030 E1031 H1032 I1033 Q1036 A1037 I1040 F1041 G1042 GLY SER GLU GLU ASN THR PRO LEU ASP LEU ASP ASP H1055 G1056 G1057 R1058 P1073 P1074 V1093 F1097 L1102 LEU VAL THR S1106
Q1107 V1126 E1127 K1128 S1129 E1130 LEU TRP VAL TYR LYS GLY GLN GLY PRO ASP GLU PRO MET ASP GLY ALA SER GLY GLU ASN GLU HIS LYS LYS THR GLU GLU GLY THR SER LYS PRO LEU LYS HIS GLU SER THR SER S1170 Y1171 N1172 Y1173 R1174 V1175 V1176 K1177 E1178 I1179 L1180 I1181 L1186
C1187 V1188 Q1189 E1190 S1191 R1195 R1198 K1199 Q1200 Q1201 Q1202 R1203 N1207 M1208 G1209 ALA HIS ALA VAL VAL LEU GLU LEU LEU GLN ILE PRO TYR GLU K1224 A1225 E1226 D1227 T1228 K1229 M1230 Q1231 E1232 I1233 M1234 L1241 C1245 A1246 Q1249 A1253 I1267 L1268 E1269 A1270 M1278 N1279
L1283 E1286 I1287 N1288 E1289 R1290 F1295 I1299 G1303 R1304 N1305 Y1308 L1312 Q1313 K1317 ALA GLU GLY LYS PHE I1323 K1324 K1325 C1326 Q1327 D1328 M1329 V1330 M1331 A1332 E1333 L1334 V1335 N1336 S1337 G1338 E1339 D1340 V1341 Y1345 N1346 D1347 R1348 A1349 T1353 L1354 I1355 Q1356 M1357 M1358
R1359 SER GLU ARG ASP ARG MET ASP GLU ASN SER PRO L1371 V1384 C1385 T1386 E1387 G1388 K1389 N1390 V1391 Y1392 T1393 E1394 I1395 K1396 C1397 N1398 S1399 L1400 L1401 P1402 L1403 D1404 V1407 R1408 V1409 V1410 T1411 H1412 E1413 D1414 C1415 I1416 P1417 E1418 V1419 K1420 I1421 A1422 N1428 H1429 C1430 Y1431 V1432 D1433 T1434
E1435 V1436 E1437 M1438 K1439 E1440 I1441 Y1442 T1443 S1444 N1445 H1446 M1447 W1448 K1449 L1450 F1451 E1452 N1453 F1454 L1455 V1456 D1457 ILE CYS ARG ALA CYS ASN ASN THR SER ASP ARG LYS HIS ALA ASP S1473 V1474 L1475 E1476 K1477 Y1478 V1479 T1480 E1481 I1482 V1483 M1484 S1485 I1486 V1487 T1488 T1489 F1490 PHE SER SER PRO
PHE SER ASP GLN SER THR THR L1502 Q1503 T1504 R1505 Q1506 P1507 V1508 F1509 V1510 Q1511 L1512 L1513 Q1514 G1515 V1516 F1517 R1518 V1519 Y1520 H1521 C1522 N1523 W1524 L1525 M1526 P1527 S1528 Q1529 K1530 A1531 S1532 V1533 E1534 S1535 C1536 I1537 R1538 VAL LEU SER ASP VAL ALA LYS SER ARG ALA ILE ALA ILE PRO VAL ASP
LEU ASP SER GLN VAL ASN ASN LEU PHE LEU LYS SER HIS ASN ILE VAL GLN LYS THR ALA MET ASN TRP ARG LEU SER ALA ARG ASN ALA ALA ARG ARG ASP SER VAL LEU ALA ALA SER ARG ASP TYR R1598 I1601 D1613 P1617 V1625 L1626 V1627 D1628 V1629 L1630 H1631 E1634
L1635 E1639 A1643 R1644 R1645 K1646 G1651 Q1662 E1666 E1669 I1673 K1674 T1678 R1687 G1688 Y1689 G1690 GLU LYS GLN ILE SER ILE ASP GLU LEU GLU ASN ALA GLU LEU PRO GLN PRO PRO GLU ALA GLU ASN SER THR GLU GLN GLU LEU GLU PRO SER PRO PRO LEU
ARG GLN LEU GLU ASP HIS LYS ARG GLY GLU GLU ALA LEU ARG GLN ILE LEU VAL ASN ARG TYR TYR GLY ASN ILE ARG PRO SER GLY ARG ARG ARG GLU SER LEU THR SER PHE GLY ASN GLY PRO LEU SER PRO GLY GLY PRO SER LYS PRO GLY GLY GLY GLY GLY PRO GLY SER GLY SER
THR S1786 R1787 G1788 E1789 M1790 S1791 V1795 G1803 A1804 S1805 I1809 T1838 S1842 D1850 K1858 D1862 T1874 V1875 T1876 T1879 SER ASP LEU GLY ASN LYS LYS LYS ASP ASP GLU VAL ASP ARG ASP ALA PRO SER ARG LYS LYS ALA LYS GLU PRO THR THR GLN ILE
THR GLU GLU VAL ARG ASP GLN LEU LEU GLU ALA SER ALA ALA THR ARG LYS ALA PHE THR THR PHE ARG ARG GLU ALA ASP PRO ASP ASP HIS TYR GLN SER GLY GLU GLY THR GLN ALA THR THR ASP LYS ALA LYS D1955 D1956 L1957 E1978 N1979 H1980 N1981 R1982 D1983 K1994 T1995 N1996
V2000 L2004 Q2005 F2006 C2009 I2010 S2013 T2014 T2015 L2018 L2021 N2026 V2030 G2062 I2063 D2064 I2065 I2066 T2067 A2068 K2079 K2080 R2081 L2084 V2085 L2088 A2092 E2110 Y2114 L2121 V2122 I2125 K2126 Y2129 E2133 V2134 E2135 F2136 E2137 D2138 G2139


E2140 N2141 G2142 E2143 D2144 G2145 G2153 Y2157 N2167 K2175 P2176 G2177 G2178 Q2179 V2180 D2181 G2182 D2183 E2184 A2185 L2186 E2187 F2188 Y2189 A2190 K2191 H2192 T2193 A2194 Q2195 R2200 L2201 D2202 R2203 E2206 F2210 P2211 V2212 P2213 S2214 I2215 C2216 E2217 F2218 L2219 T2220 K2221 E2222 S2223 K2224 L2225 R2226 I2227
Y2228 Y2229 T2230 T2231 E2232 R2233 Q2236 G2237 S2238 K2239 I2240 N2241 D2242 F2243 F2244 L2245 R2246 S2247 E2248 D2249 L2250 F2251 N2252 E2253 M2254 N2255 W2256 Q2257 K2258 K2259 A2262 V2265 L2266 Y2267 W2268 C2269 A2270 R2271 N2272 M2273 S2274 F2275 W2276 S2277 S2278 I2279 S2280 F2281 N2282 L2283 A2284 V2285 L2286 M2287 N2288 L2289 L2290
V2291 A2292 F2293 F2294 Y2295 K2298 G2299 V2300 R2301 G2302 L2305 GLU PRO HIS TRP SER GLY LEU LEU TRP THR ALA MET LEU ILE SER LEU LEU ALA ILE VAL ILE ALA LEU PRO LYS PRO HIS GLY ILE ARG A2335 L2336 I2337 A2338 S2339 T2340 I2341 L2342 R2343 L2344 I2345 F2346 S2347 V2348 G2349 L2350 Q2351 P2352
T2353 L2354 F2355 L2356 L2357 G2358 N2361 V2362 C2363 N2364 K2365 I2366 I2367 F2368 L2369 M2370 S2371 F2372 C2376 G2377 T2378 F2379 T2380 R2381 G2382 Y2383 R2384 V2387 L2388 E2391 F2392 L2393 Y2394 H2395 L2396 L2397 Y2398 L2399 L2400 I2401 C2402 A2403 M2404 G2405 L2406 F2407 V2408 H2409 E2410 F2411 F2412 Y2413 S2414 L2415 L2416 L2417
F2418 D2419 L2420 V2421 Y2422 R2423 E2424 E2425 T2426 V2434 L2443 I2450 L2451 V2452 Y2453 L2454 F2455 S2456 I2457 V2458 G2459 Y2460 K2464 D2465 D2466 F2467 I2468 L2469 E2470 VAL ASP ARG LEU PRO ASN GLU THR ALA GLY PRO GLU THR GLY GLU SER LEU ALA ASN ASP PHE LEU TYR SER ASP VAL CYS
ARG VAL GLU THR GLY GLU ASN CYS THR SER PRO ALA PRO LYS GLU GLU LEU LEU PRO VAL GLU E2519 T2520 K2524 E2525 H2526 T2527 C2528 E2529 T2530 T2537 V2538 L2539 S2540 H2541 R2544 S2545 G2546 G2547 G2548 V2549 G2550 D2551 V2552 L2553 R2554 E2560 F2563 A2564 A2565 R2566 V2567 I2568 Y2569 D2570
L2571 L2572 F2573 F2574 F2575 M2576 V2577 I2578 I2579 I2580 V2581 L2582 N2583 L2584 T2585 F2586 G2587 V2588 I2589 E2599 K2600 Q2601 K2602 I2606 T2609 T2610 C2611 F2612 I2613 C2614 G2615 L2616 E2617 R2618 D2619 K2620 F2621 D2622 N2623 K2624 T2625 V2626 T2627 F2628 E2629 E2630 H2631 I2632 K2633 E2634 E2635 H2636 N2637 M2638 W2639 H2640
V2646 K2649 V2650 K2651 D2652 E2655 Y2656 T2657 G2658 P2659 E2660 S2661 Y2662 E2665 M2666 I2667 R2670 N2671 L2672 F2675 M2678 M2681 S2682 L2683 V2684 S2685 S2686 D2687 S2688 E2689 G2690 E2691 Q2692 N2693 E2694 L2695 R2696 N2697 L2698 Q2699 E2700 E2703 S2704 T2705 M2706 K2707 L2708 V2709 T2710 N2711 L2712
Q2715 L2716 S2717 E2718 L2719 K2720 D2721 Q2722 M2723 R2727 K2728 Q2729 K2730 Q2731 R2732 I2733 G2734 L2735 L2736 G2737 H2738 P2739 PRO HIS MET ASN VAL ASN PRO GLN GLN PRO ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	65438	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.961	Depositor
Minimum map value	-8.843	Depositor
Average map value	0.082	Depositor
Map value standard deviation	0.673	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	252.0, 252.0, 252.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.57	8/13005 (0.1%)	0.95	73/17078 (0.4%)
1	B	0.57	8/13005 (0.1%)	0.95	73/17078 (0.4%)
1	C	0.57	8/13005 (0.1%)	0.95	73/17078 (0.4%)
1	D	0.57	8/13005 (0.1%)	0.95	73/17078 (0.4%)
All	All	0.57	32/52020 (0.1%)	0.95	292/68312 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	B	0	25
1	C	0	25
1	D	0	25
All	All	0	100

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	629	ARG	C-O	6.61	1.35	1.23
1	C	629	ARG	C-O	6.58	1.35	1.23
1	A	629	ARG	C-O	6.57	1.35	1.23
1	D	629	ARG	C-O	6.54	1.35	1.23
1	B	2336	LEU	C-O	6.22	1.35	1.23

The worst 5 of 292 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2554	ARG	N-CA-C	12.32	144.26	111.00
1	B	2554	ARG	N-CA-C	12.31	144.24	111.00
1	A	2554	ARG	N-CA-C	12.31	144.24	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	2554	ARG	N-CA-C	12.30	144.20	111.00
1	B	1278	MET	N-CA-C	11.50	142.05	111.00

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	LYS	Peptide
1	B	249	LYS	Peptide
1	B	260	GLN	Peptide
1	B	393	LEU	Peptide
1	B	65	ARG	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12851	0	9511	1261	0
1	B	12851	0	9511	1263	0
1	C	12851	0	9511	1263	0
1	D	12851	0	9511	1266	0
All	All	51404	0	38044	4698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

The worst 5 of 4698 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2618:ARG:HD2	1:C:2628:PHE:CZ	1.25	1.71
1:A:538:LEU:CG	1:A:586:GLY:HA2	1.25	1.67
1:A:2618:ARG:HG3	1:A:2628:PHE:CE1	1.17	1.67
1:D:2618:ARG:HG3	1:D:2628:PHE:CE1	1.17	1.67
1:B:2618:ARG:HD2	1:B:2628:PHE:CZ	1.25	1.66

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2132/2750 (78%)	1860 (87%)	235 (11%)	37 (2%)	9	43
1	B	2132/2750 (78%)	1862 (87%)	233 (11%)	37 (2%)	9	43
1	C	2132/2750 (78%)	1860 (87%)	235 (11%)	37 (2%)	9	43
1	D	2132/2750 (78%)	1861 (87%)	234 (11%)	37 (2%)	9	43
All	All	8528/11000 (78%)	7443 (87%)	937 (11%)	148 (2%)	13	43

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	588	ASP
1	B	1073	PRO
1	B	1074	PRO
1	B	1190	GLU
1	B	1199	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	921/2459 (38%)	785 (85%)	136 (15%)	3	18
1	B	921/2459 (38%)	786 (85%)	135 (15%)	3	19
1	C	921/2459 (38%)	785 (85%)	136 (15%)	3	18
1	D	921/2459 (38%)	785 (85%)	136 (15%)	3	18
All	All	3684/9836 (38%)	3141 (85%)	543 (15%)	6	19

5 of 543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2336	LEU
1	C	2388	LEU
1	C	2294	PHE
1	C	2649	LYS
1	A	2351	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2637	ASN
1	C	2252	ASN
1	D	2693	ASN
1	C	289	HIS
1	C	2395	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

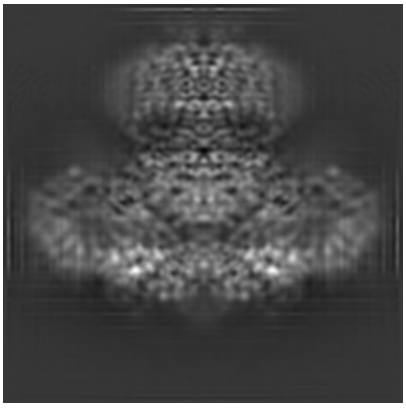
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9244. These allow visual inspection of the internal detail of the map and identification of artifacts.

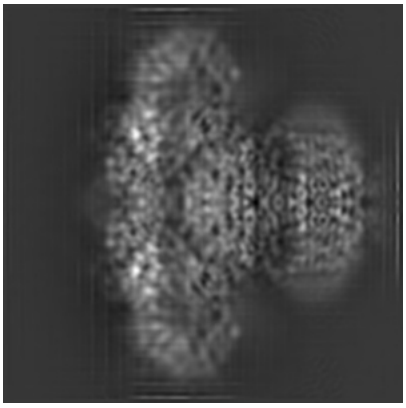
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

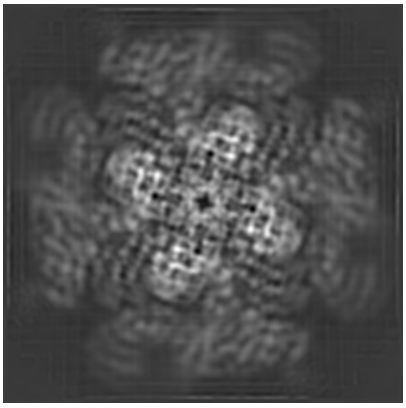
6.1.1 Primary map



X



Y



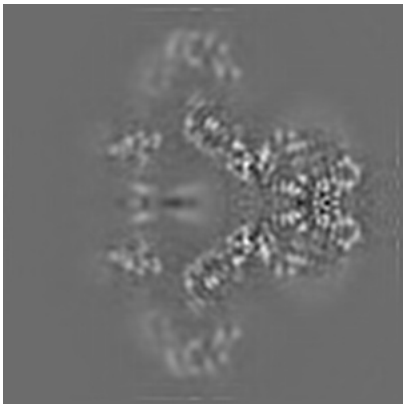
Z

The images above show the map projected in three orthogonal directions.

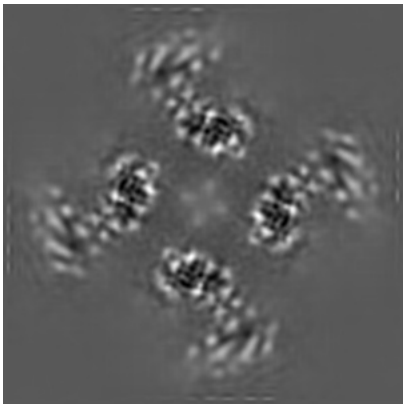
6.2 Central slices (i)

6.2.1 Primary map

X Index: 100



Y Index: 100

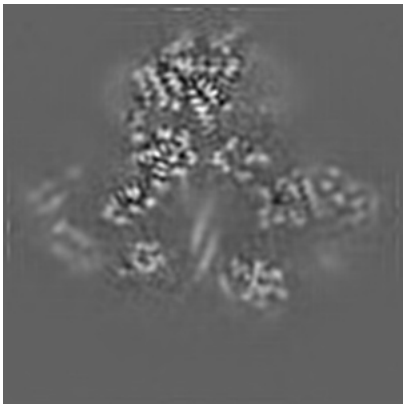


Z Index: 100

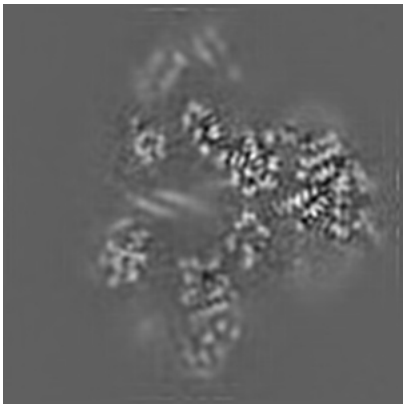
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

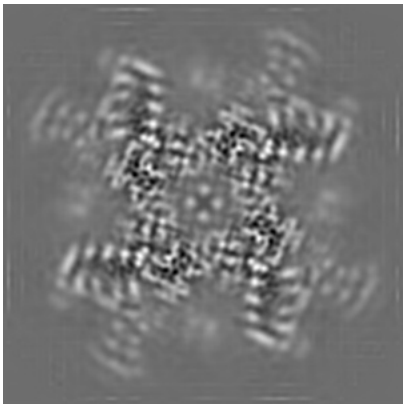
6.3.1 Primary map



X Index: 94



Y Index: 94



Z Index: 70

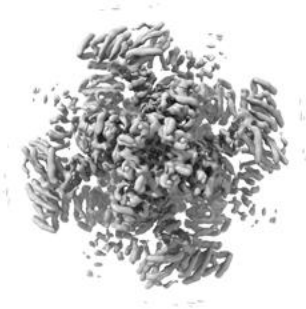
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

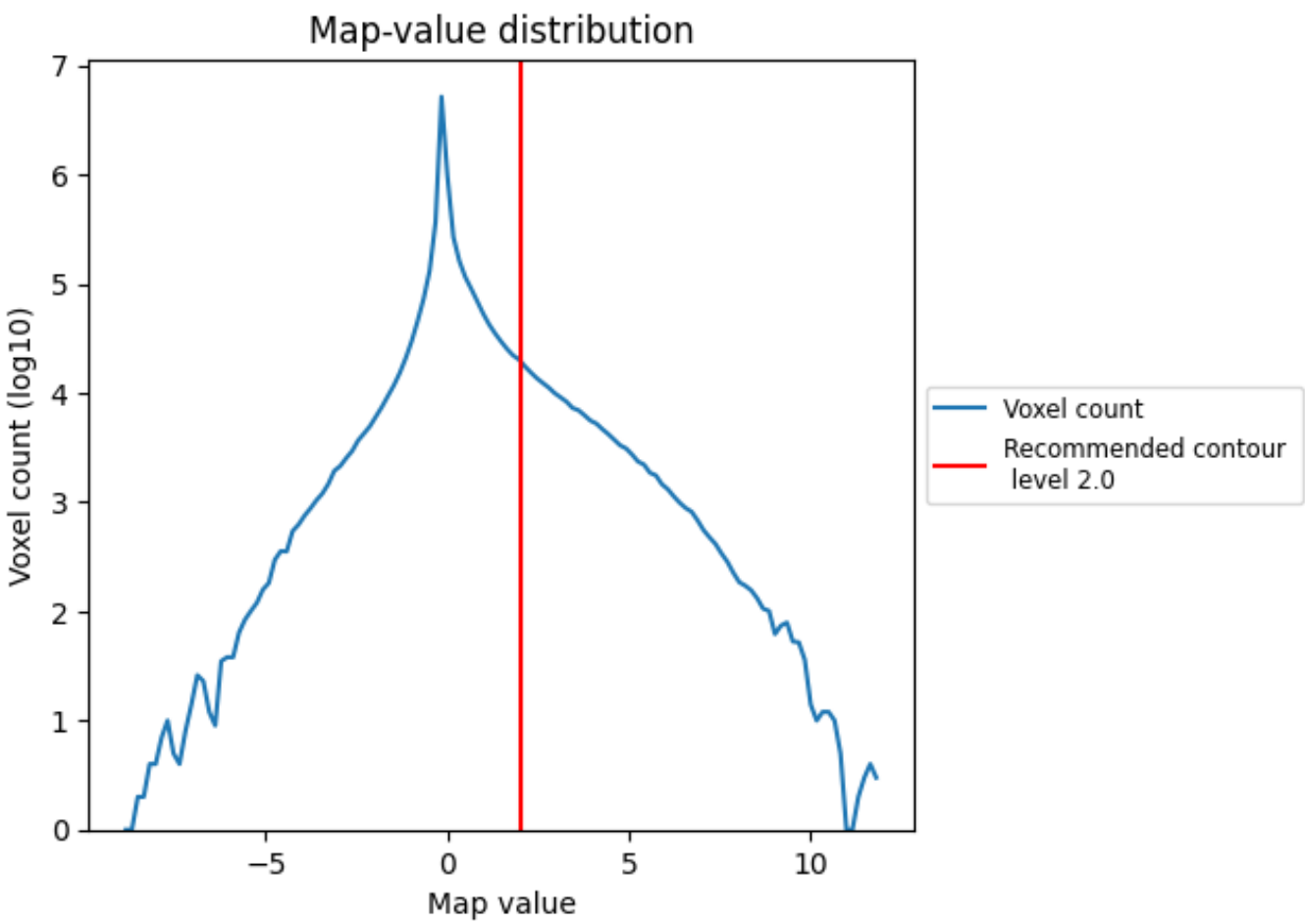
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

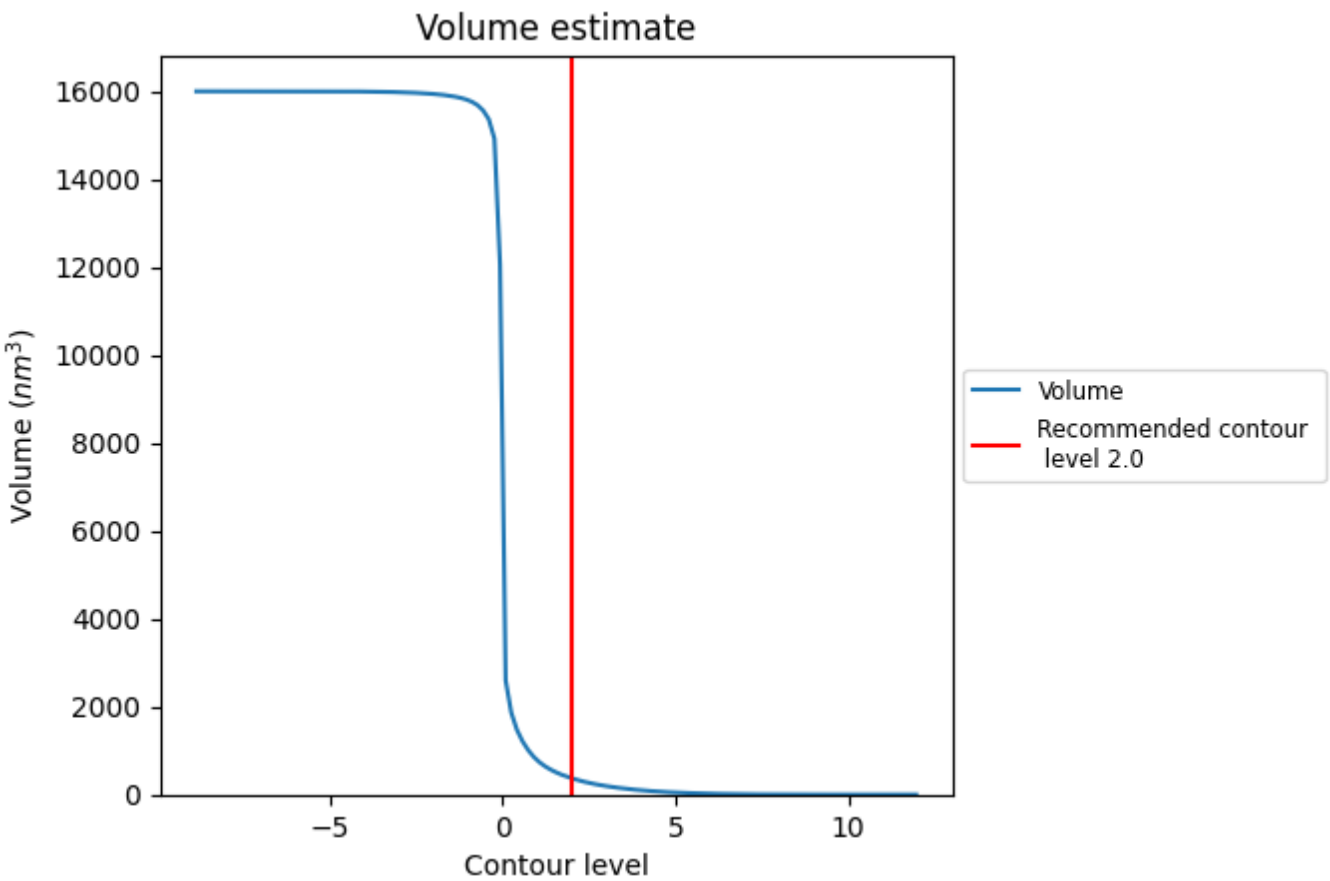
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

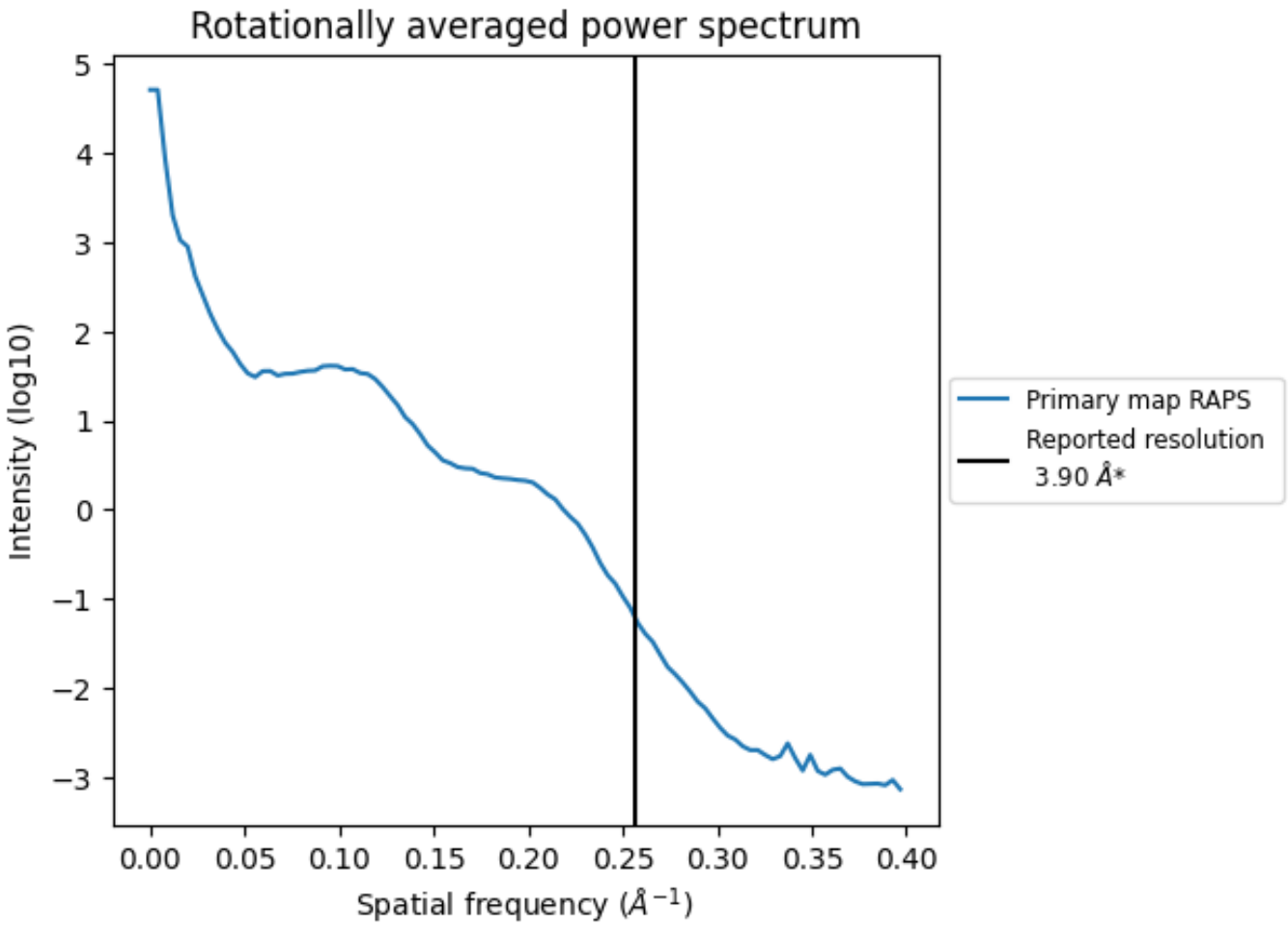
7.2 Volume estimate (i)



The volume at the recommended contour level is 372 nm^3; this corresponds to an approximate mass of 336 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

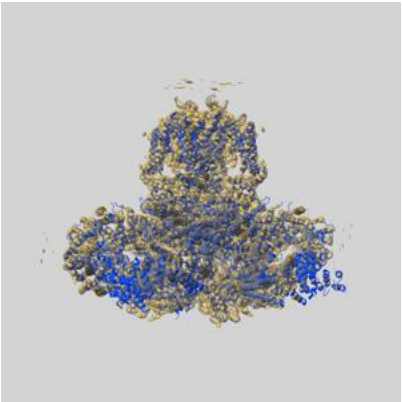
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

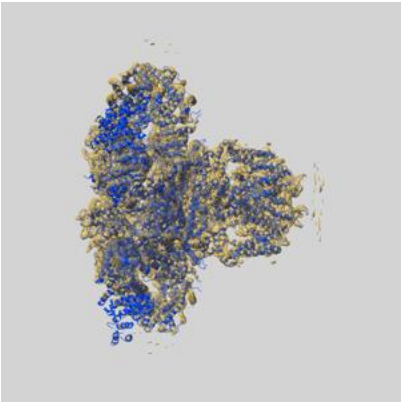
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9244 and PDB model 6MU2. Per-residue inclusion information can be found in section 3 on page 4.

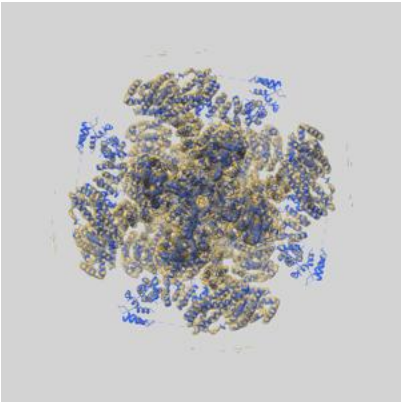
9.1 Map-model overlay (i)



X



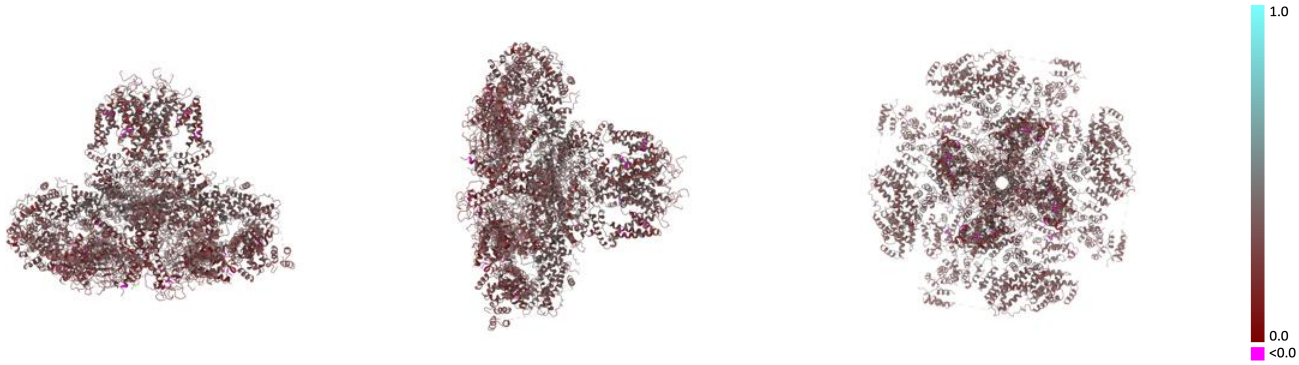
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

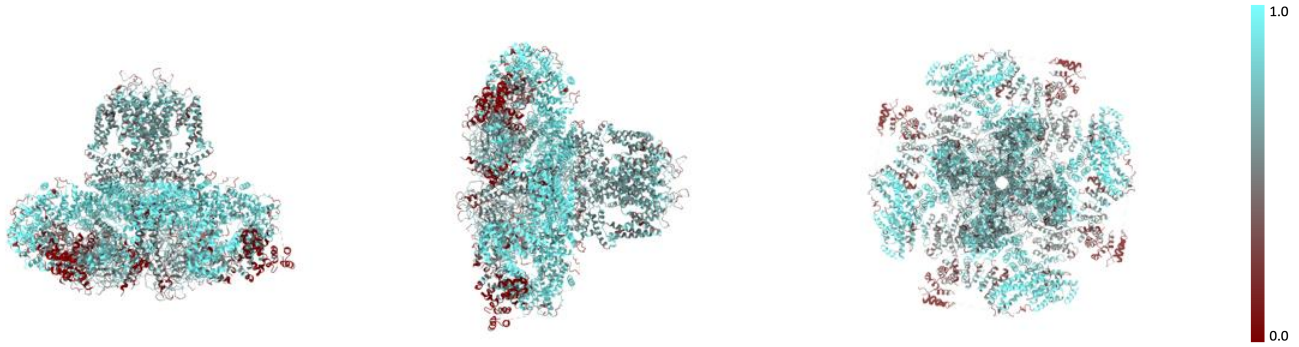
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

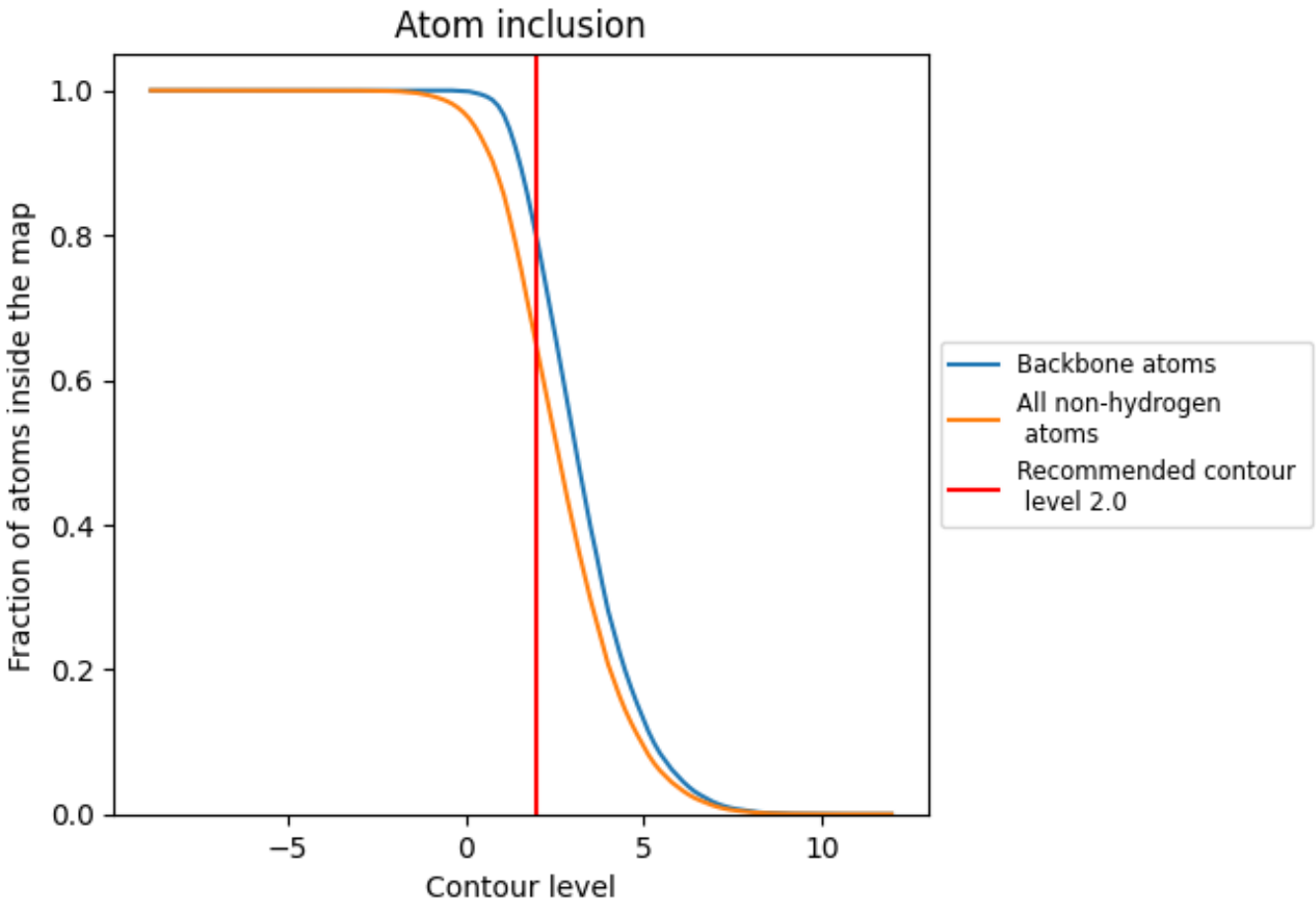
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6435	0.3100
A	0.6439	0.3100
B	0.6447	0.3100
C	0.6435	0.3100
D	0.6421	0.3080